Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.12

Global applicability domain: Inside

Local applicability domain index: 6.14e-01

Confidence level: 6.38e-01

Nearest Neighbors from the Training Set

Image not found
Propane, 2-methyl-1-nitro-
Measured: 1.40
Predicted: 1.42

Image not found
Propane, 2-methyl-2-nitro-
Measured: 1.17
Predicted: 1.33

Image not found
1-Nitrobutane
Measured: 1.47
Predicted: 1.35

Image not found
1-Nitropentane
Measured: 2.01
Predicted: 1.83